

Advanced Photon Source Update

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APS Users Organization & Partner User Council Joint Meeting

July 9, 2014

Overview

- Science Highlights
- Recent Reviews
- DOE Triennial Review and Strategic Planning
- Budget
- Other Business: End of Experiment Forms, Hosting



Neurotransmitter-Receptor Structures Provide Insight on Brain Function

Scientific Achievement

Determination of x-ray crystal structures of two challenging membrane proteins provide functional insight on ionotropic and metabotropic glutamate receptors in molecular detail

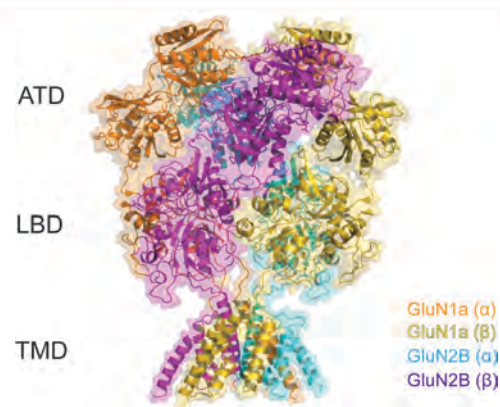
Significance and Impact

Glutamate receptors are pharmaceutical targets for brain disorders including Alzheimer's disease, Parkinson's disease, depression, schizophrenia, autism, and ischemic injuries associated with stroke

Research Details

- Fast-acting, ionotropic glutamate receptor structure reveals a putative calcium binding site, which may be pivotal for neuronal plasticity
- Long-acting, metabotropic glutamate receptor (a GPCR) structure reveals binding site of an allosteric drug candidate

Work was performed at Argonne National Laboratory



Structure of a heterotetrameric NMDA receptor ion channel: the dimer of heterodimers shows the amino-terminal domain (ATD), ligand-binding domain (LBD), and transmembrane domain (TMD).

E. Karakas and H. Furukawa, "Crystal structure of a heterotetrameric NMDA receptor ion channel," *Science* **344**, 992 (May 30 2014). DOI:10.1126/science.1251915
Contact: furukawa@cshl.edu



Artistic view of a human metabotropic glutamate receptor 1: a negative allosteric modulator is shown bound to the transmembrane domain on the left; a dimer, including the extra-cellular domain, is shown at right.

H. Wu, C. Wang, K.J. Gregory, G. W. Han, H.P. Cho, Y. Xia, C.M. Niswender, V. Katrich, J. Meiler, V. Cherezov, P.J. Conn, R.C. Stevens, "Structure of a Class C GPCR Metabotropic Glutamate Receptor 1 Bound to an Allosteric Modulator," *Science* **344**, 58 (2014). DOI: 10.1126/science.1249489

Contact: stevens@scripps.edu

X-ray Magnetic Diffraction to Record High Pressure

Scientific Achievement

X-ray magnetic diffraction and band structure modeling revealed a robust organization between itinerant, local spins in maintaining antiferromagnetism over 13% volume change

Significance and Impact

Direct insight of magnetic order in single-crystal samples provided by x-rays to highest pressure to date using newly designed experimental techniques

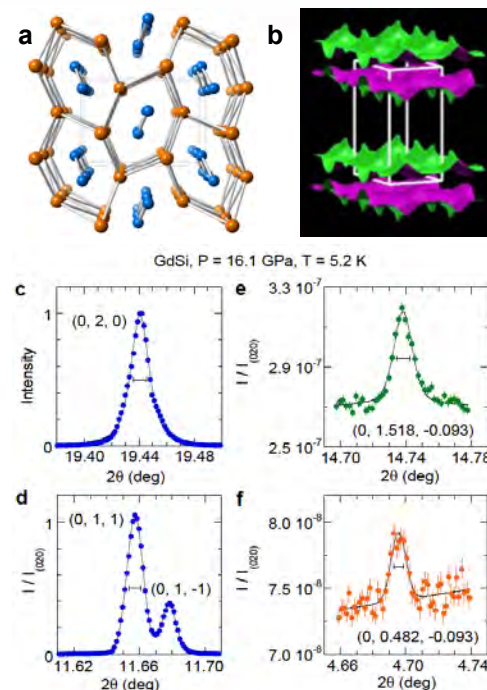
Research Details

- X-ray magnetic diffraction used to directly probe antiferromagnetism under pressure to 17 GPa
- Magnetic order was attributed to cooperative interaction between local and itinerant spins in the rare-earth intermetallic compound
- Band structure calculation provides insight into origin of magnetic stability under pressure, as a persistently nested Fermi surface grows increasingly one-dimensional in this three-dimensional metal

Y. Feng, J. Wang, A. Palmer, J. A. Aguiar, B. Mihaila, J.-Q. Yan, P. B. Littlewood, T.F. Rosenbaum, in press, *Nature Communications* (2014).

Contact yejun@aps.anl.gov

Work performed at Argonne National Laboratory



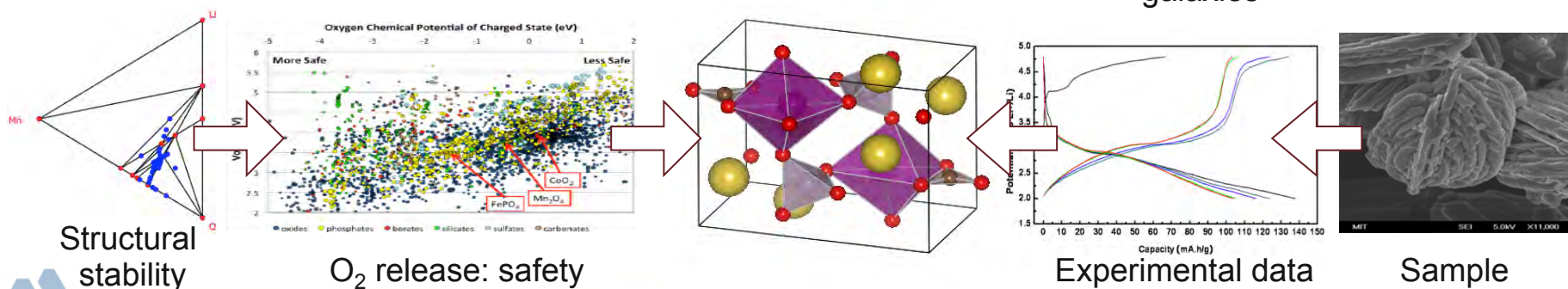
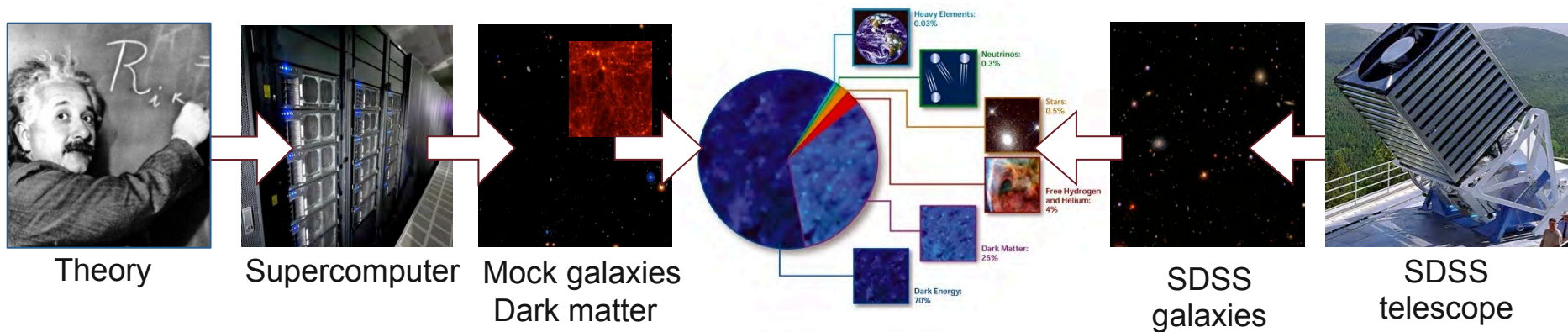
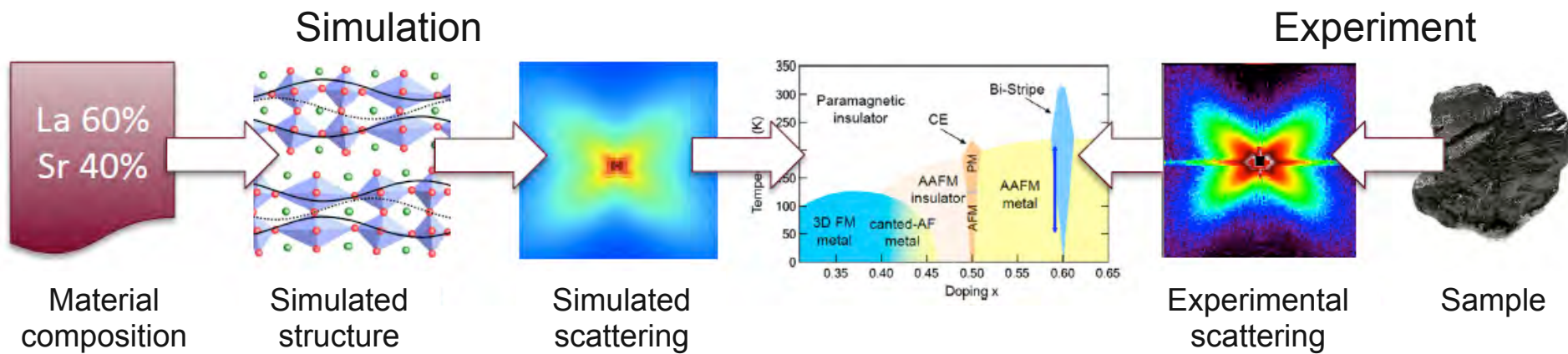
X-ray magnetic diffraction of spin-density wave antiferromagnetism in GdSi under pressure: (a) The lattice structure of GdSi shows a hidden one-dimensional order. (b) Calculated nesting Fermi surface at 16.1 GPa, where diffraction signals of lattice (c-d) and magnetism (e-f) were observed. X-ray diffraction provides unprecedented high resolution at such high pressure.


Recent Reviews: It's Been a Busy Two Months!

- The University of Chicago Argonne, LLC **Board of Governors Annual Review** of the Photon Sciences Directorate and Advanced Photon Source was held May 28-30.
 - “This review will focus on the facility’s accelerator/user operations and scientific productivity in preparation for the DOE Triennial Review to be held in June 2014.”
- Argonne annual **Lab Plan Presentation** to the Department of Energy on June 11.
- **Quarterly Board of Governors Meeting** held on June 18 – 19 focused on APS-U.
- Argonne’s strategy presented to Secretary of Energy Ernie Moniz and the **Secretary of Energy Advisory Board** on June 19.
 - “The Board will provide advice and recommendations to the Secretary of Energy on the Department’s basic and applied research and development activities, economic and national security policy, educational issues, operational issues, and on any other activities and operations of the Department of Energy as the Secretary may direct.”
- The **DOE Triennial Review of the APS** was held June 24-27.



Message to Secretary of Energy Advisory Board: Bringing Big Data and Simulation Together





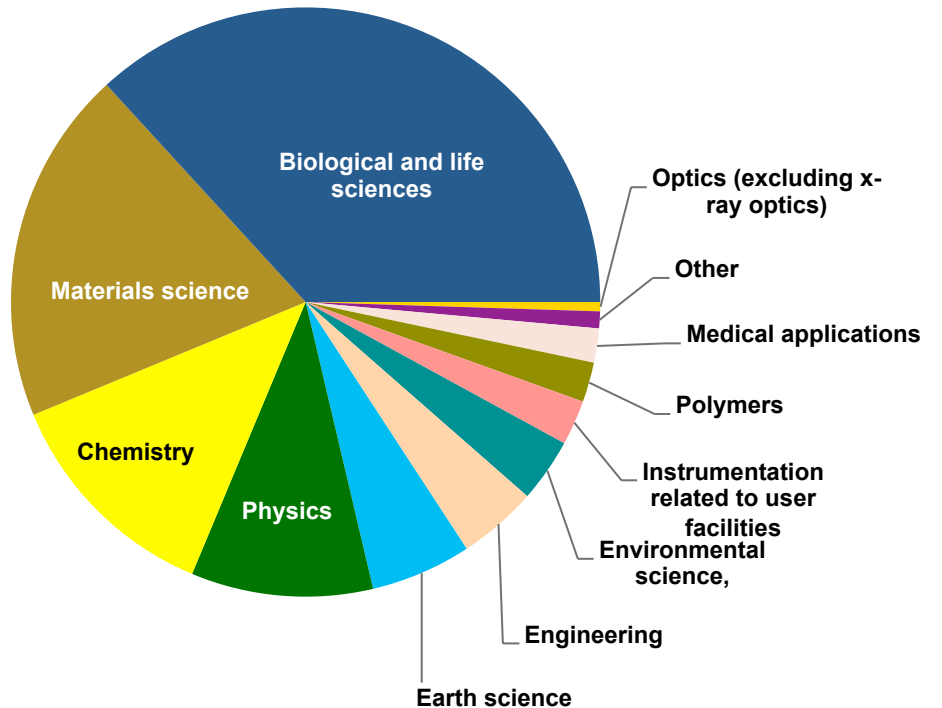
The DOE Triennial Review: Strategy, Strategy, and Strategy And Budget



The APS Has a Successful Record of Productivity and Growth

- High brightness and flux at high energies
- “Short” pulses, high rep rate, flexible bunch structure
- Wide array of beamlines, beam time available for complex experiments
- Large and diverse community
- Integrated with other Argonne strengths

- Life Sciences: ~40% of experiments
- Physical Sciences: ~60% of experiments

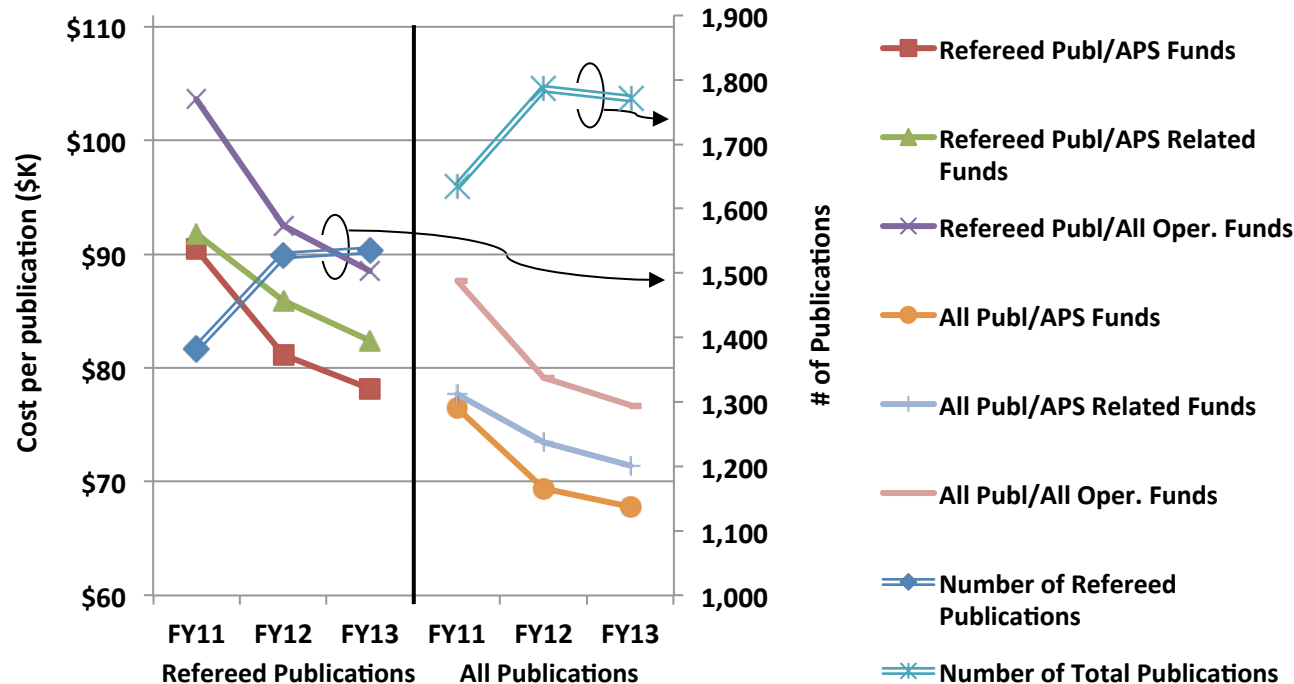


- >24,000 visits up from 22,500 by 5,728 users (+7%)
- 5,200 experiments in FY13, up from 4,900 (+6%)
- 1,771 total publications in CY13, up from 1,530 (+16%); 29% high impact
- >98% beam availability
- Over 1,500 protein structure deposits in CY13



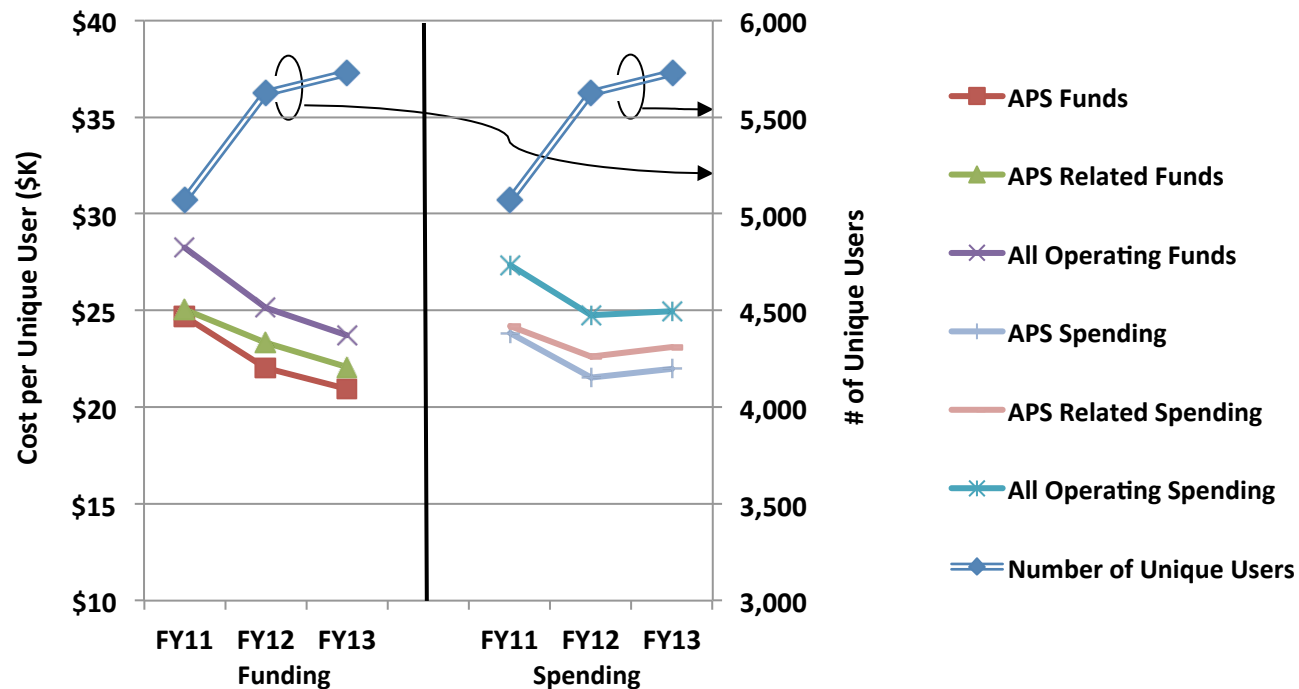
Publication Metrics:

Cost/Publication Continues to Improve



- Papers are by calendar year
- Three metrics:
 1. APS Operating Funds – Operating funding provided by BES-SUF for support of APS
 2. Related Operating Funds – Metric #1 plus recovery from proprietary research and NIH/GM-CA
 3. All Operating Funds – Metric #2 plus operating funds from all other sources. Excludes the Upgrade and DCS Projects and ARRA equipment funds.
- Two perspectives: refereed publications and all publications

Publication Metrics: Cost/Unique User Has Improved, But...



- Same three metrics
- Views with number of publications based on funding and spending
- Unique users include on-site and off-site users

Accelerator Performance Is Outstanding

FY11-13 Mean Time Between Faults (MTBF): 128.8 hours

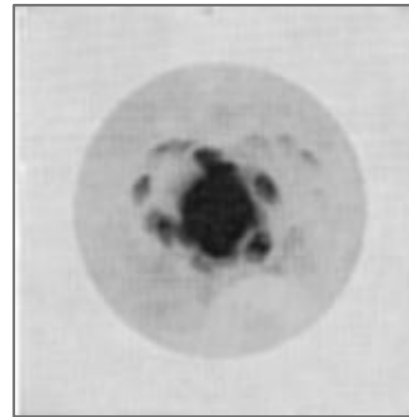
FY11-13 Availability: 98.5%

FY14 To Date: MTBF 121.9 hrs, Availability 98.3%

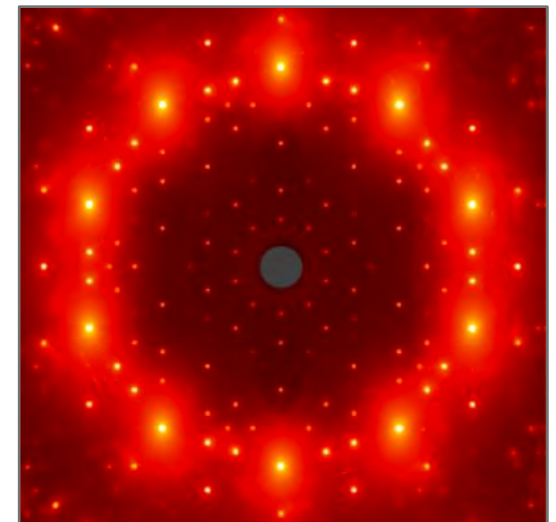
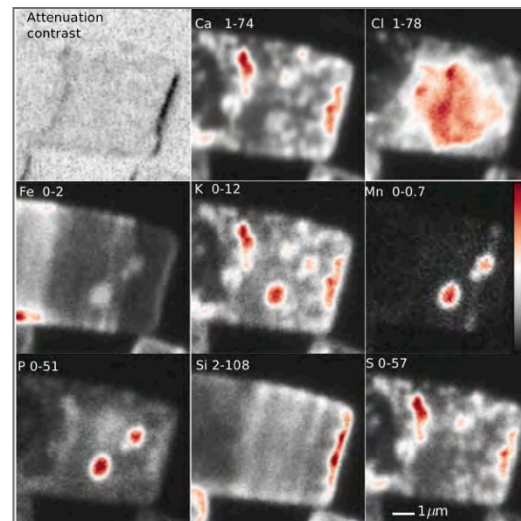
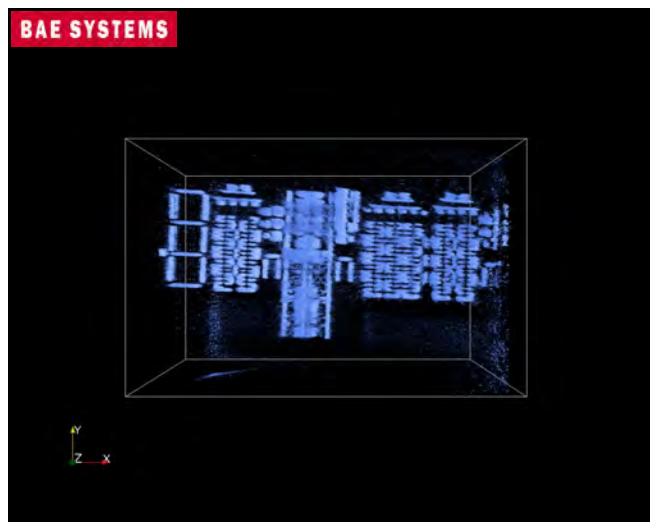
Made possible by proactive accelerator team and QA program



Where Next? Uniting the Worlds of Roentgen and von Laue

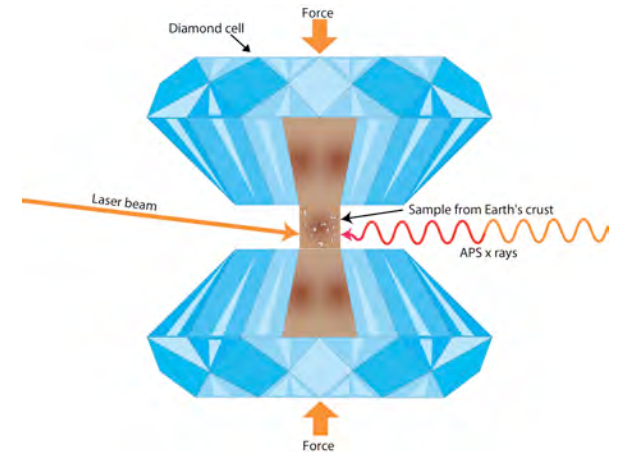


- Imaging yield submicron information
- Diffraction yields sub-nanometer information

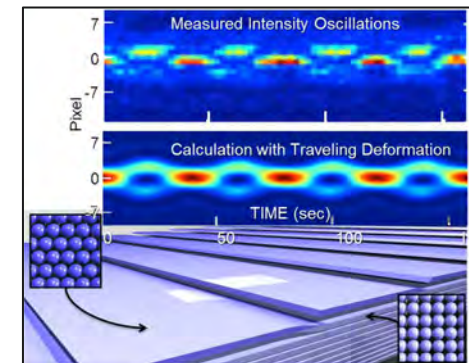


Exploits APS' Future Source Characteristics: High Energy Brightness, Coherence, and Nanobeams

- High resolution, real time exploration of *in operando* or *in situ* phenomena: exploring engineered systems and chemical processes
- Science at terascale pressures
- Structure and chemistry of individual nano-objects: beyond ensemble measurements
- Structure and dynamics in non-periodic systems
- Nanoscale imaging and spectroscopy of collective behavior in inhomogeneous systems
- Structure and dynamics of cellular machinery
- Trace element migration and evolution in environmental and biological systems



To exceed today's limit of 400 MPa,
need higher flux
to see signals from small samples



Increased coherence for better time and
spatial resolution

Our Challenge: Develop a Strategic Plan that Achieves APS Goals and Allows Us to Prioritize Investments

- Provide the world-leading high-brightness hard x-ray user facility to enable outstanding science by users (including staff)
- Upgrade the APS with state-of-the-art technology to maintain world leadership
- Enable continued progress in light sources and their utilization
- Assure the safety of the facility users and staff and the environment
- Maintain a world-class organization that is diverse, inclusive, and focused on innovation. Provide a rewarding environment for staff and users that fosters professional growth.

Work with User Communities and Partners to position ourselves for an upgraded APS, and to make use of the APS-U Installation Period



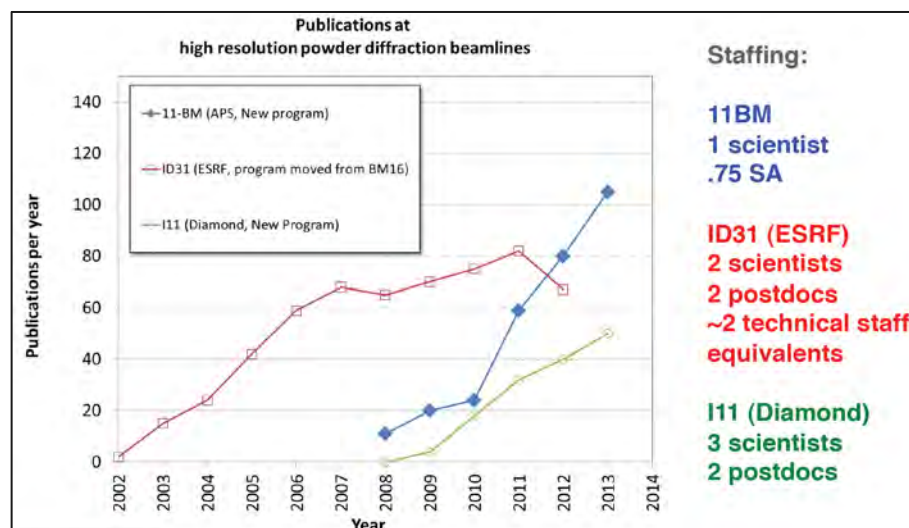
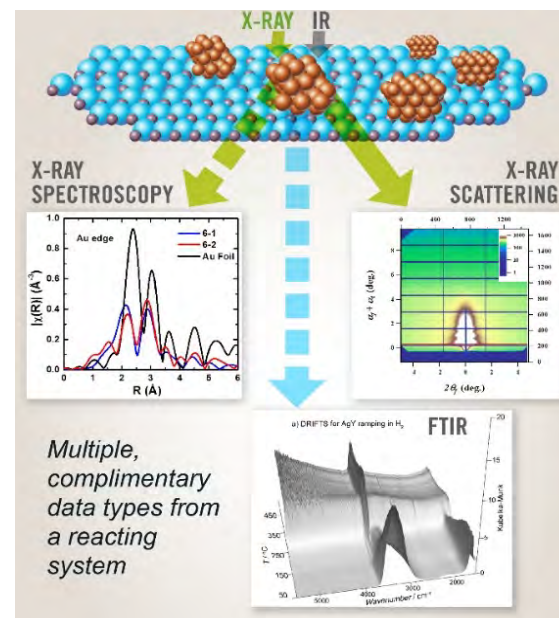
APS Will Achieve Its Goals By Investment in Well-Defined Areas

- X-ray operations
- Accelerator operations
- Improvements
- Staff science supporting the APS mission
- Mission readiness
- Strategic research and development
- Infrastructure, general operations, and administration
- Human capital and workforce development
- We will also engage in special projects and Work for Others that are consistent with our mission, strengths, and goals



X-ray Operations: Enabling the User Community

- Accommodate NSLS users during transition
- Increase efficiency and throughput: automation and remote access
- Expand multi-modal characterization capabilities
 - Distributed access Raman spectrometer
 - HEDM+tomography, USAXS+SAXS+WAXS
- Build on the success of the detector pool



Detector Pool

The Detectors Group operates the APS Detector Pool.

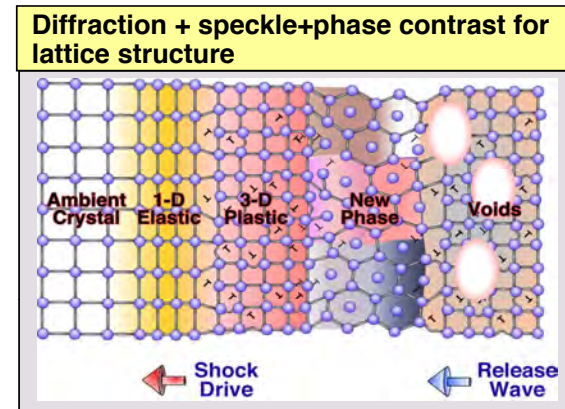
Submit a Detector Request

Detector Pool staff can be contacted during normal work hours / run period Monday-Friday at 2-9490 or for general questions dp@aps.anl.gov

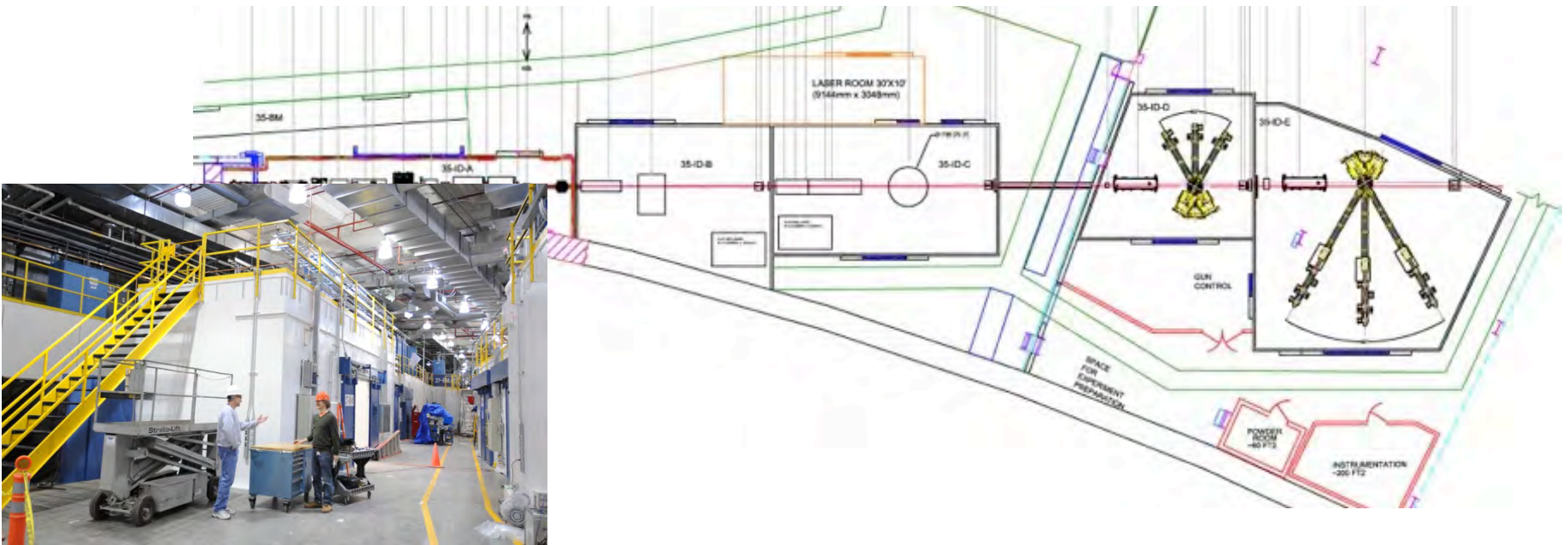


FY15: Finish Moving Beamlines to Operation

- Intermediate Energy X-ray (IEX) 29-ID
 - NSF/DOE funded, APS to operate
- Resonant Inelastic X-ray Scattering (RIXS) 27-ID
 - APS-U funded, APS to operate
- High-Energy Diffraction 6-BM
 - COMPRES/NSLS/APS to operate
- Dynamic Compression Sector (DCS) 35-ID
 - NNSA funded, WSU to operate



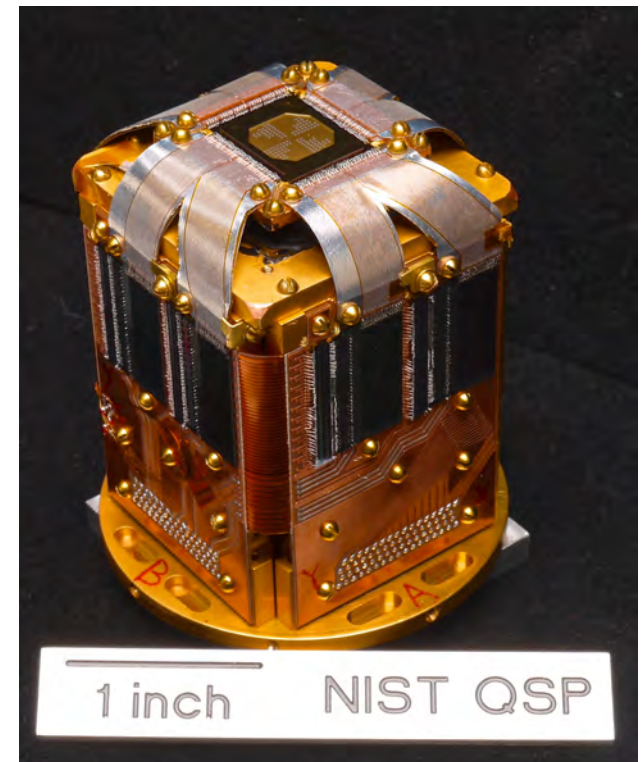
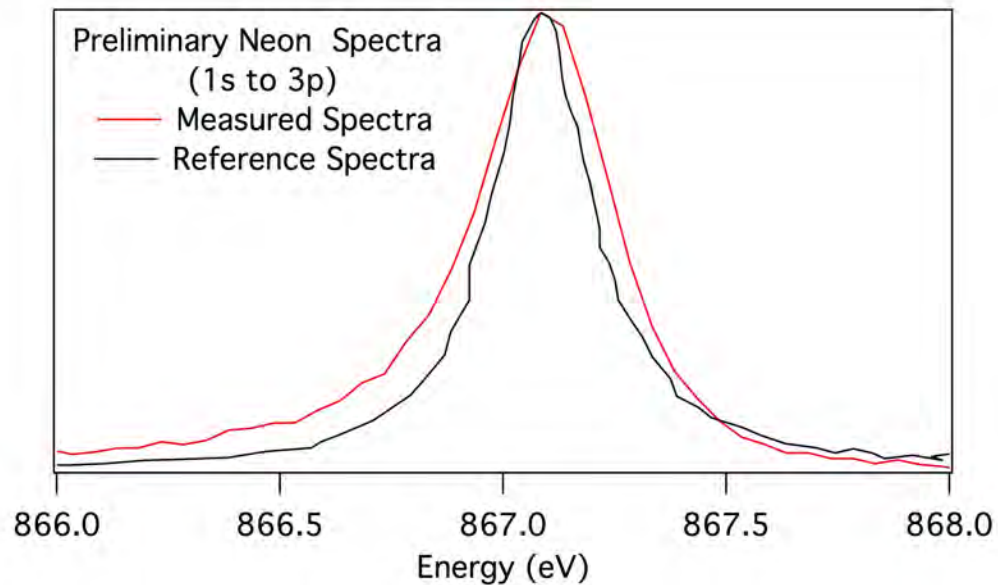
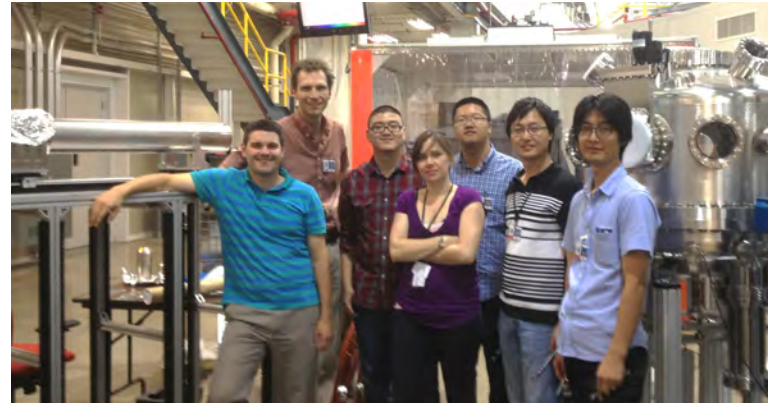
R. Collins, LLNL



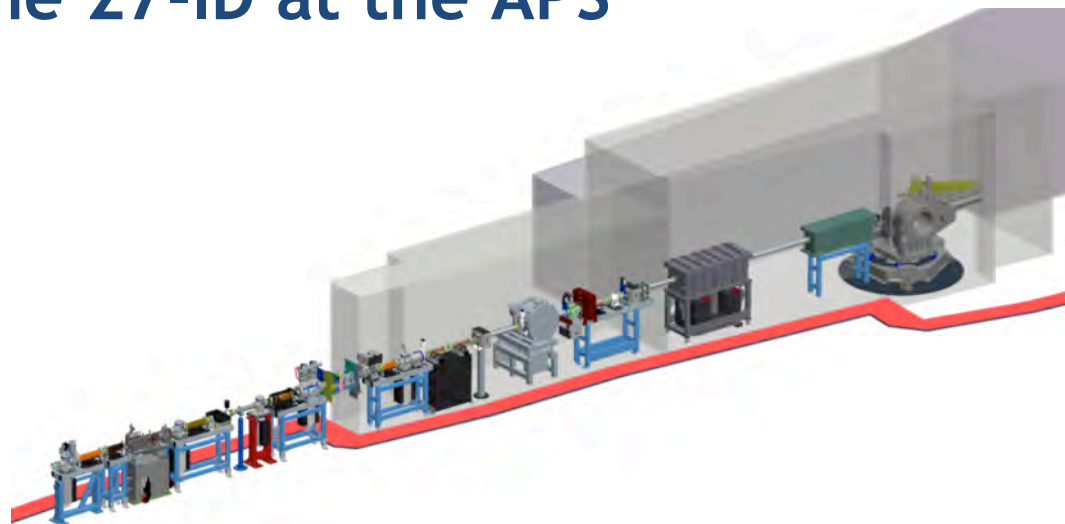
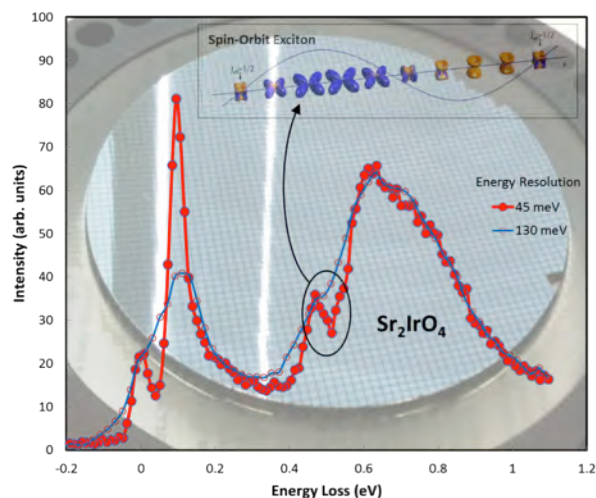
IEX Status Update

- Currently commissioning beamline optics
- Refocusing optics being installed
- Endstations in construction
- Expected first measurements 2014-3 cycle

TES detector installation



The New Resonant Inelastic X-ray Scattering (RIXS) Beamline 27-ID at the APS



Dedicated, Optimized State-of-the-Art Insertion Device Beamline Offering

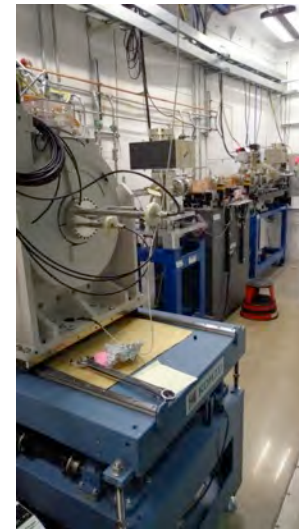
- **Unprecedented Energy-Resolution**, Comparable to Inelastic Neutron Scattering (5 ... 10 meV) at Highest X-ray Intensities
- **Advanced Focusing and In-Situ Sample Environments**
- Consolidation of all RIXS Activities at the APS on one Beamline

MBA lattice will Further Enhance Focusing and Energy-Resolution



Construction Status of 27-ID (July 1st, 2014)

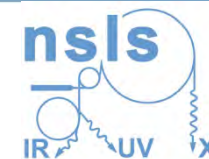
- All conventional facilities (Shielding Enclosures, Control Room, Utilities ...) are finished
- Shielding verification for 27-ID-A has been completed (**first photons on this brand-new beamline**), small radiation leaks have been mitigated
- All First-Optics-Enclosure components are installed (white-beam slit, monochromator, white-beam stop, collimators, photon shutter, ...)
- Beamline vacuum is being established
- **First monochromatic beam expected third week of July, 2014**
- Installation of RIXS instrumentation expected for September, 2014
- Commissioning and limited user operations in 2014-3 and 2015-1



Upstream and downstream – views of inside of FOE

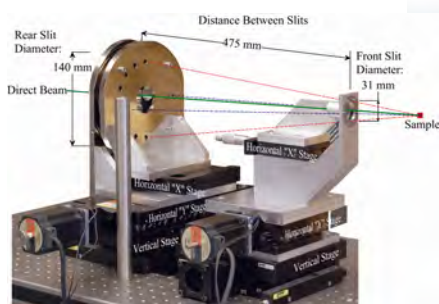


6-BM: White beam energy dispersive diffraction



6-BM-B:

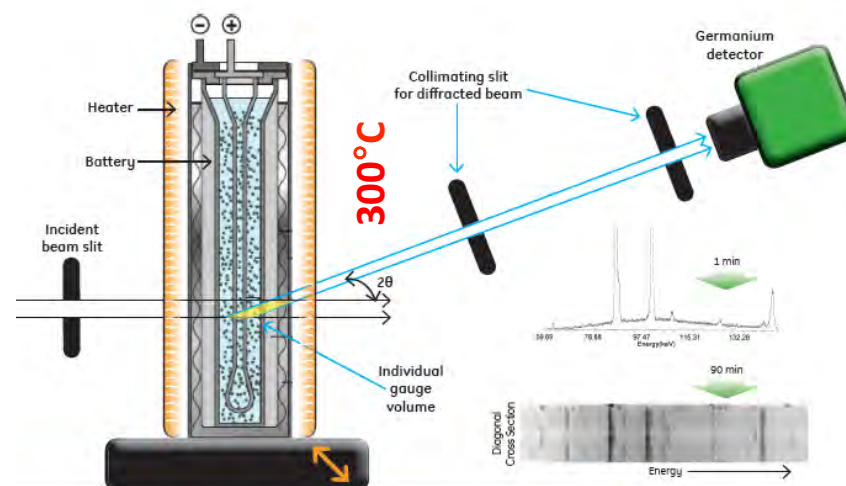
Large Volume Press – High Pressure EDD



COMPRES – High pressure earth sciences consortium

6-BM-A:

General EDD – Spatially resolved XRD



Sample stage

GE Global Research, Rutgers University, BNL, Engineering/Battery research

HP-EDD (50%) – Supported by COMPRES (via Stony Brook) with one resident full time staff

General – EDD – 17% reserved for NSLS Engineering battery research supported by NSLS staff, remainder supported by MPE group (50% XSD staff).

NSLS EDD group and XSD MPE group having bi-weekly teleconference calls to plan for move. Commissioning in Fall 2014 with full operations expected in Feb 2015

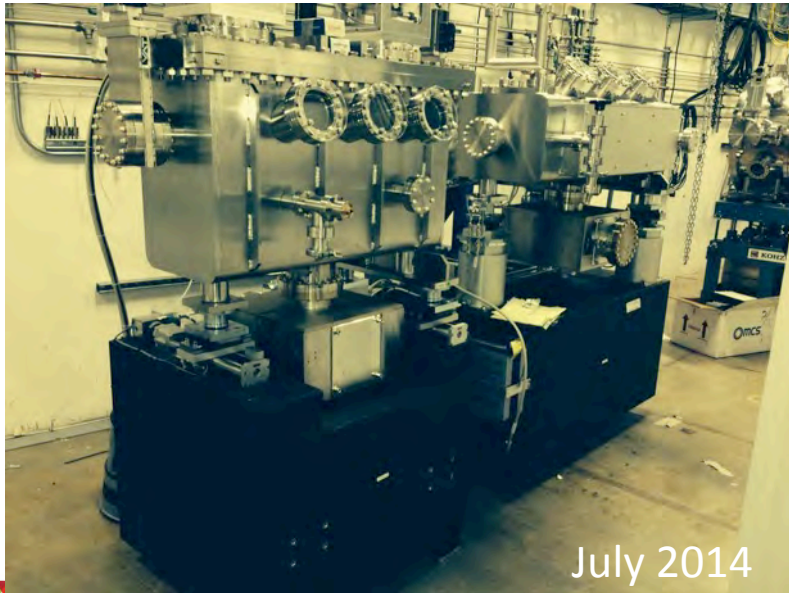


Dynamic Compression Sector Construction Progress

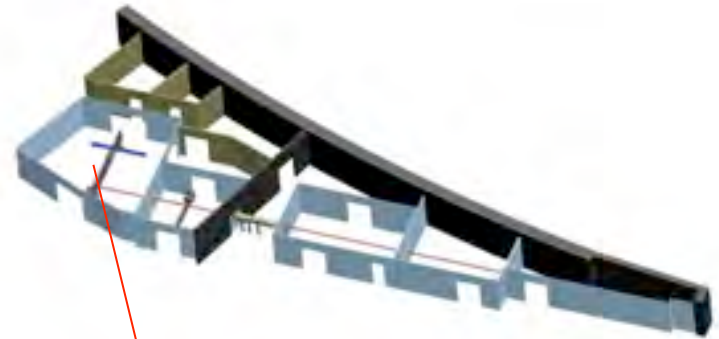


March 2014

Focusing mirrors



July 2014



Two-stage gun installation
in 35-ID-E



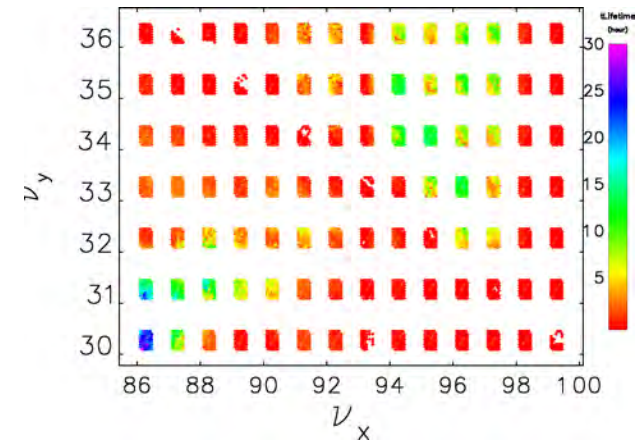
July 2014



Accelerator Operations: Advancing Machine Performance

- Continue development and improvement of accelerator simulation codes and capabilities, and partner with other parts of ANL and outside organizations to gain access and contribute to state-of-the-art computational methods.
- Use the existing APS storage ring and injector accelerators for benchmarking theory and simulation.
- Implement diagnostic system upgrades aimed at meeting or exceeding beam stability goals for the MBA upgrade. These include improvements to the electron and x-ray beam position monitors, beam size monitors, and the real-time orbit feedback system.
- Develop novel undulators including permanent-magnet and superconducting undulators, and fast switching electromagnet undulators

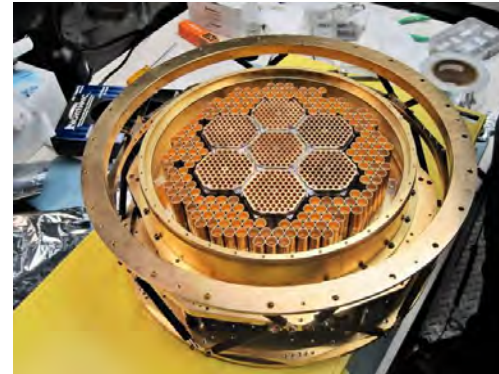
Use of HPC to perform wide- ranging analysis of Touschek lifetimes with APS codes



New Fast Feedback

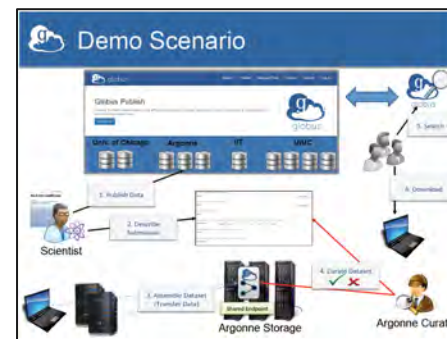
Strategic R&D Directions

- Beamlines and Experimental Techniques that will Exploit APS-U
- Optics
- Detectors
- Nanopositioning
- Sample Environments
- Data and Analysis
- Magnetic Devices
- Beam Stability
- Enabling Time-Resolved Research for the APS Upgrade
- Sources beyond APS-U



ANL will build all 15,200 sensors for SPT-3G

- Detectors: Leverage initiative between Argonne and University of Chicago
 - Large area photodetectors
 - Superconducting bolometric detectors for the South Pole Telescope (SPT)
 - Quantum engineering
 - **Future detector technologies for the APS**



*Ian Foster, et al.,
(Argonne and U.
Chicago),
Globeus – Publishing and
Discovery Demo, Globeus
World 2014*

- Leverage Argonne expertise in exascale computing , data and computational science applications

Optics: new Modular Mirror/Multilayer Deposition

- Goal 1: Mirror refurbishment. Existing mirrors up to 1.5 m long, ion milling for figure error correction, *in situ* measurement of figure errors, profiled ion beam milling for figure correction. Cost efficient for this mission alone!
- Goal 2: Highly efficient multilayer monochromators, graded multilayer mirrors for focusing and collimation.
- Goal 3: Thin film R&D (including multilayer Laue lenses for nanofocusing) with improved velocity stability, sputtering targets, partial pressure gas control. Best path to sub-10 nm nanofocusing at selected energies.
- *In situ* metrology – no removal & remounting of mirror – different than, e.g., Thales SESO
- 12" planar cathodes (BNL has 3" diameter; less growth rate drift).
- Precision multiple reactive gas mixing.
- *In situ* metrology capable
- Dynamic aperture capable (3-D film gradients)



\$1.3 M + \$0.5 M interferometer;
will replace 20 year old system

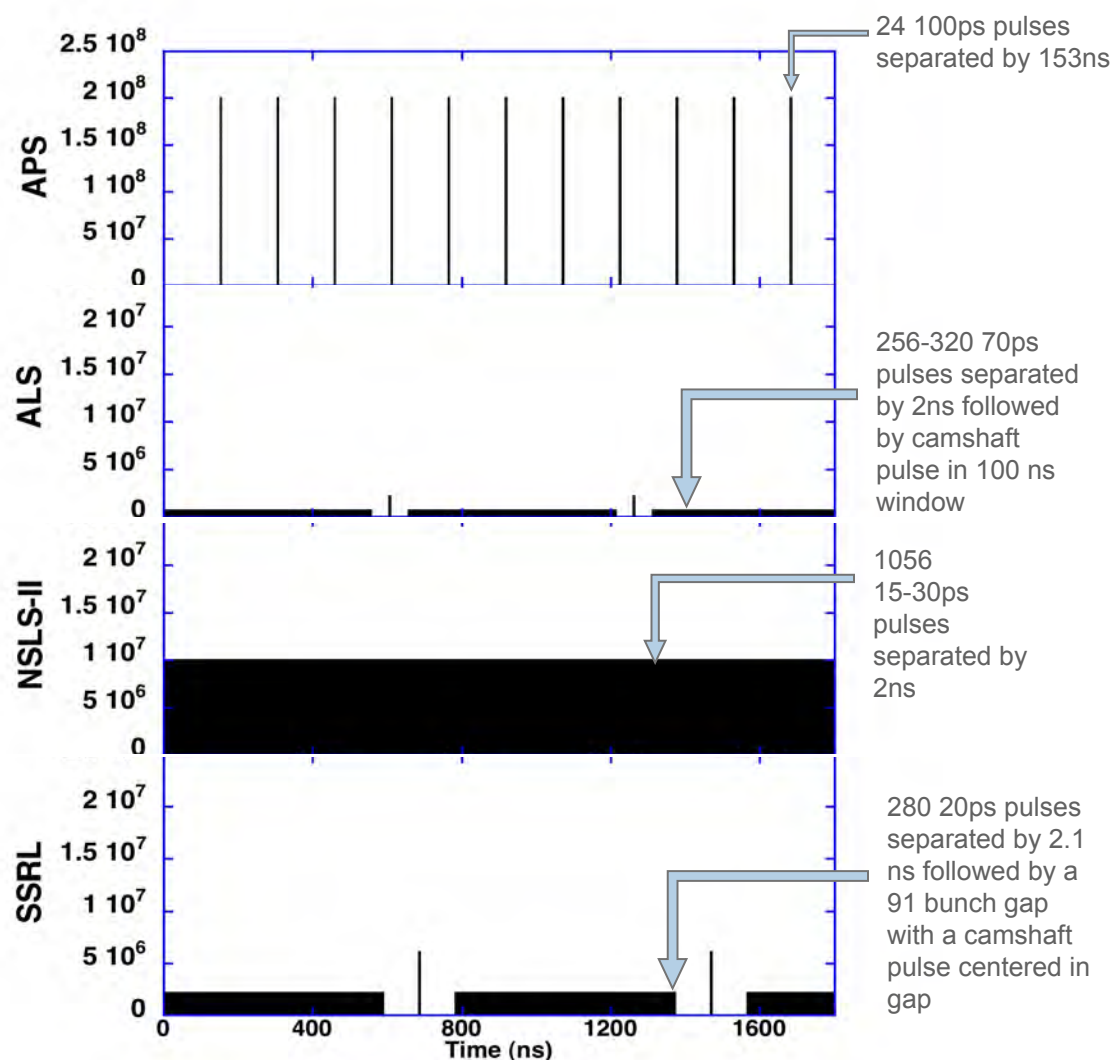
Detector R&D Initiatives

- **Superconducting energy dispersive detectors**
 - Target application: chemical imaging (XES) at scanning nanoprobe
 - Seeded by DOE Early Career Grant
 - APS & HEP teams are increasing the level of integration (“Argonne Detector Center”)
 - Joint ANL-NIST-SLAC proposal being written for DOE/SUF
- **Integrating pixel detectors (“FASPAX”)**
 - Target application: pump-probe-probe-probe .. diffraction
 - Pump-probe crystallography (Sector 14) & Dynamic compression (Sector 35)
 - Movies of dynamic processes with a burst frame rate of 13 MHz.
 - Collaboration with Fermilab
 - APS-Upgrade funded (for the moment)
- **Sparsified pixel detectors for XPCS (“VIPIC”)**
 - Target application: Microsecond time-tagged photon readout for ultra-fast XPCS
 - First synchrotron tests of prototype scheduled for July 2014 at 8-ID
 - Joint ANL-BNL-FNAL proposal being written for DOE/SUF
 - Deliver two 1-Megapixel detectors for APS and NSLS-2
- **Germanium strip detectors**
 - Target applications: Energy-dispersive diffraction and high-energy powder diffraction
 - EDD programs at 6-BM, 1-BM, and 13-BM
 - Collaboration with BNL (Siddons)
 - APS ALD provided seed funding (\$50k)
 - Joint ANL-BNL proposal being written for DOE/SUF



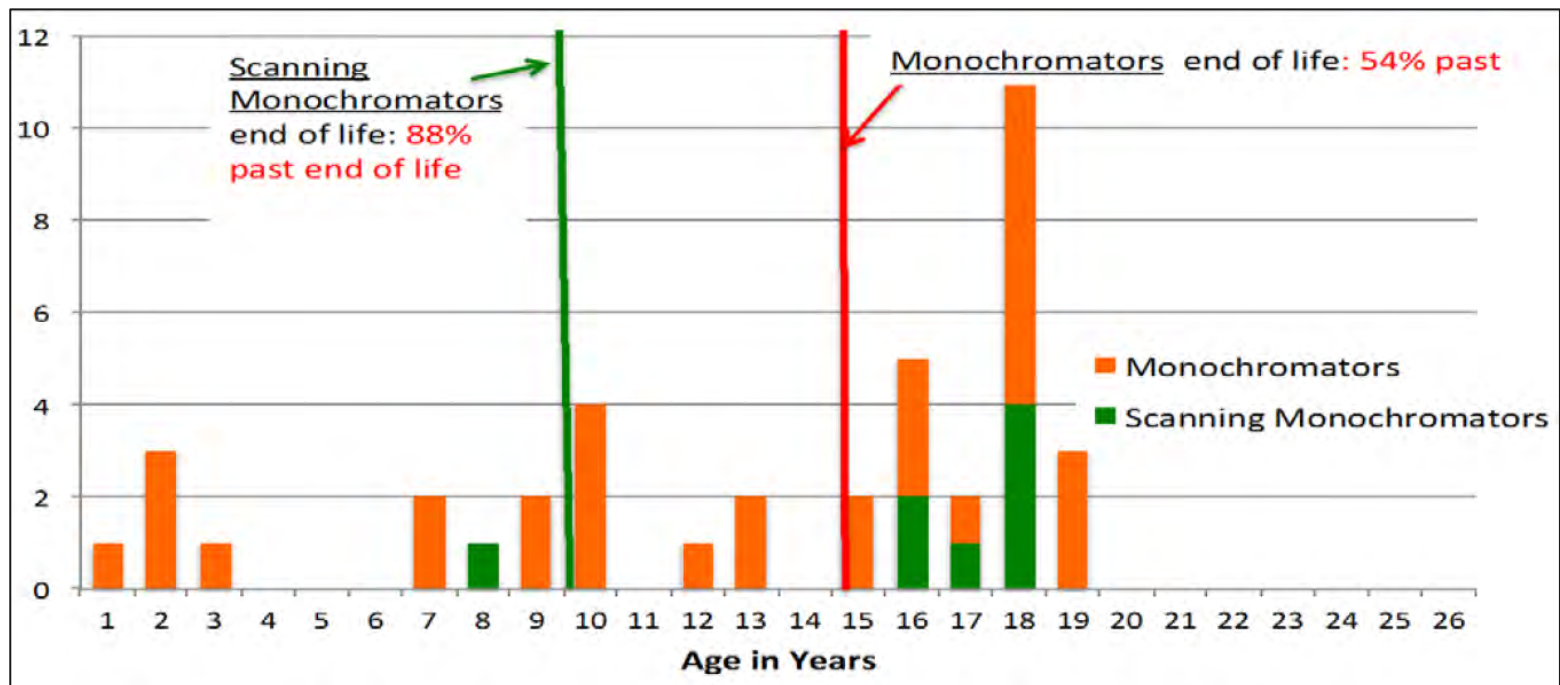
Enabling Time-Resolved Research for the APS Upgrade

- R&D on technologies and experimental methods to isolate individual x-rays pulses from the expected 48-bunch, 200-mA fill pattern for an upgraded APS
- R&D on increasing the current per bunch in a 24-bunch fill pattern for an upgraded APS, to increase total current above 100 mA



Invest in Mission Readiness Across the Facility

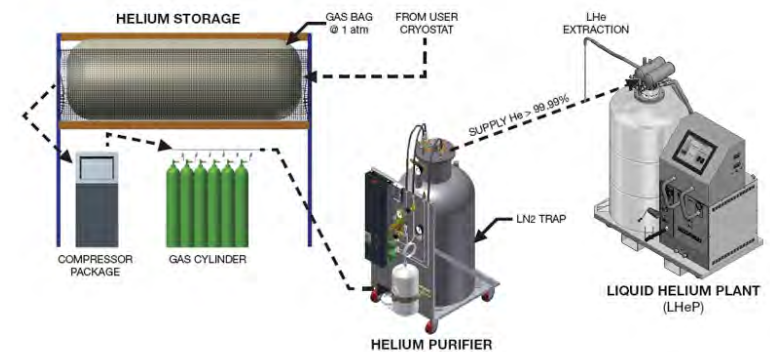
- Develop a comprehensive plan to anticipate and mitigate risks associated with beamline and accelerator equipment reliability, end-of-life failure, and obsolescence.
- Applied to all work that is not included in the scope of the APS Upgrade project but is required for the long-term reliable operation of APS.
- Includes beamline systems
- Began approx. 6 months ago



Infrastructure, General Operations, and Administration

- Opportunities to increase efficiency, reduce consumables costs
- Improve user processes and scientific access
- Ensure access to required engineering and staging facilities
- Improve APS experimental hall environmental stability
- Upgrade Argonne campus network infrastructure

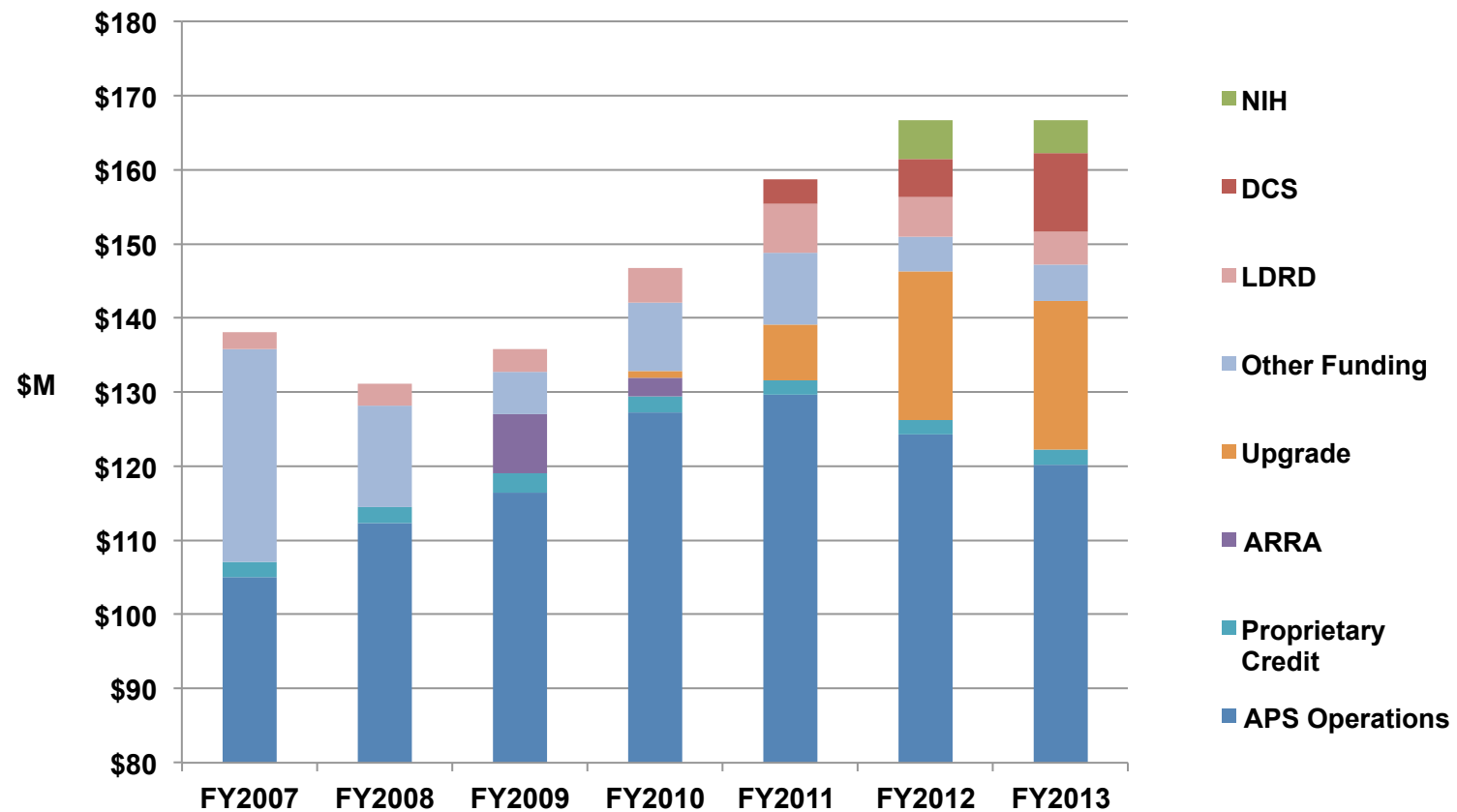
Helium Recovery System



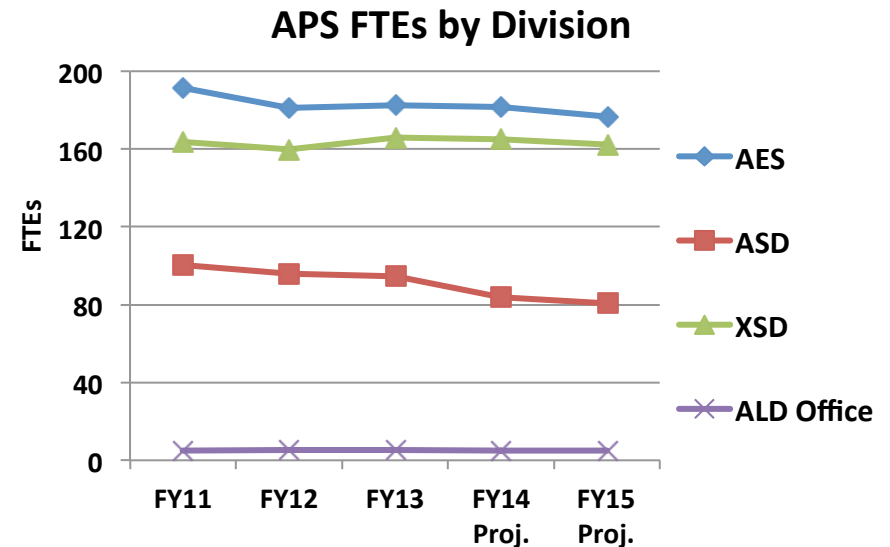
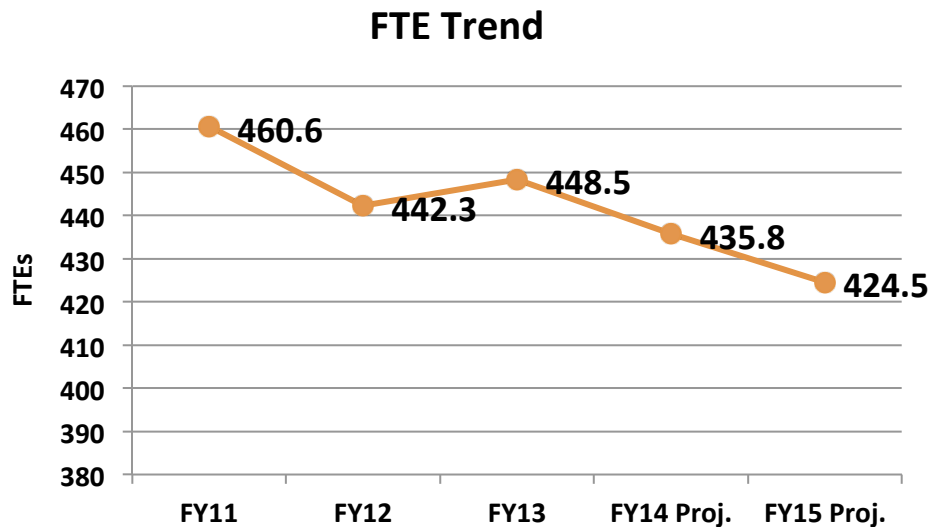


Budget: Efficiency, Investment for the Future with Flat or Declining Budgets

Photon Sciences Funding



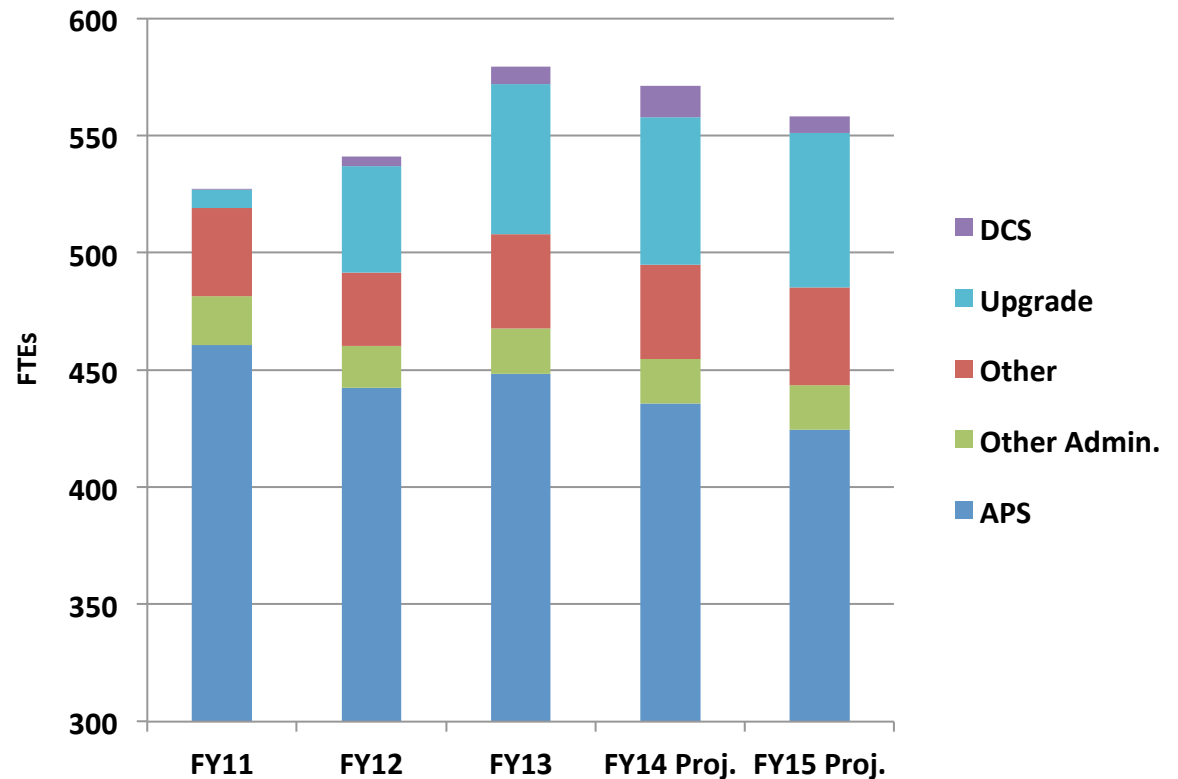
APS Operations Staffing Optimization: Trend Towards More Efficiency



- Reduction in force: 30 staff; full cost savings not until FY15
- Number of Special Term Appointees (STA) use reduced
- Eliminated 9 contractors

FTE Future Trend

- Lean staffing level of APS Operations
- Reduction in APS FY14 & FY15 staffing depicts the full value of the recent reduction in force
- DCS Project scheduled for completion in mid-FY15.



FY15 Funding Outlook

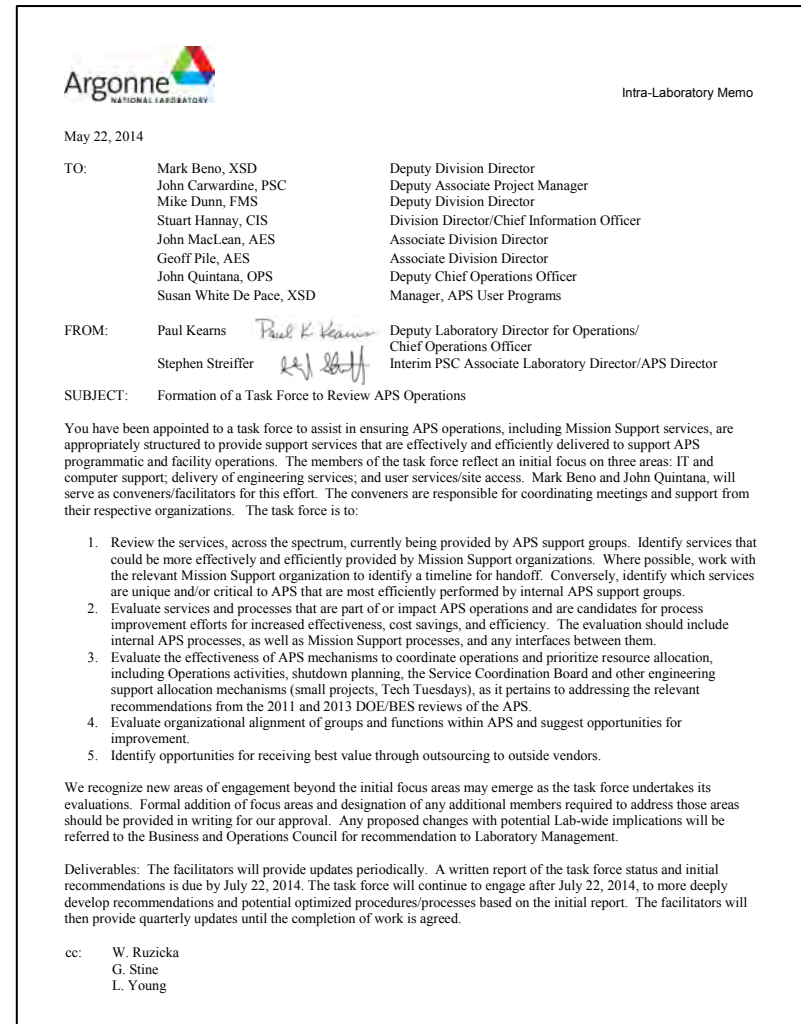
Office of Science (SC)

ITEM	FY12 Conf.	FY13 Enacted	FY14 Omnibus	FY15 Request	FY15 House	FY15 Senate
SC						
ASCR:	442,000	440,825	478,593	541,000	541,000	
BES:						
Research	1,542,600	1,538,498	1,610,757	1,667,800	1,574,000	
<u>Construction</u>	<u>151,400</u>	<u>150,997</u>	<u>102,000</u>	<u>138,700</u>	<u>128,000</u>	
Total BES	1,694,000	1,689,495	1,712,757	1,806,500	1,702,000	
BER:	611,823	610,196	610,196	628,000	540,000	
FES:						
Research			305,677	266,000	315,000	
<u>Constr. ITER</u>			<u>200,000</u>	<u>150,000</u>	<u>225,000</u>	
Total FES	402,177	401,108	505,667	416,000	540,000	
HEP:						
Research	763,700	761,669	746,521	738,000	738,000	
<u>Construction</u>	<u>28,000</u>	<u>27,926</u>	<u>51,000</u>	<u>25,000</u>	<u>37,000</u>	
Total HEP	791,700	789,595	797,521	744,000	775,000	
NP:						
Research	---	498,670	489,438	487,073	493,500	
<u>Construction</u>	<u>---</u>	<u>49,867</u>	<u>80,500</u>	<u>106,500</u>	<u>106,500</u>	
Total NP	550,000	548,537	569,938	593,573	600,000	
SLI:	111,800	111,503	97,818	79,189	79,189	
S&S:	82,000	81,782	87,000	94,000	94,000	
Workforce:	18,500	18,451	26,500	19,500	19,500	
Prog. Dir.:	185,000	184,508	185,000	189,393	180,000	
<u>Resc. /Pr. Yr.</u>	<u>---</u>	<u>---</u>	<u>---</u>	<u>---</u>	<u>---</u>	
Total	4,889,000	4,876,000	5,071,000	5,111,155	5,071,000	5,086,000



We must deliver more scope for the dollar

- Senior management will conduct a top-down assessment of organization and efficiencies
- A working group will evaluate several aspects of APS operations, organization, and interactions with central Argonne support services. The task force includes both key APS and Argonne mission support leaders.
- We will gather input from experimental-floor-level staff on what they believe is working and what is not.





Other Business: End of Experiment Forms, Hosting



End-Of-Experiment Forms

Pat Dehmer – “Great Science, Happy Users”

- A mechanism to have rapid feedback from users for desired improvements.
- APS recently revamped (Oct 2013) EEFs to allow for beamline specific questions.
- Used to spot trends and allocate resources to trouble spots
- Who reads the EEFs? Principal Beamline Scientist, Group Leader, (mgmt has access)
- Incorporating a beamline scientist additional comment feature.

Some remarks:

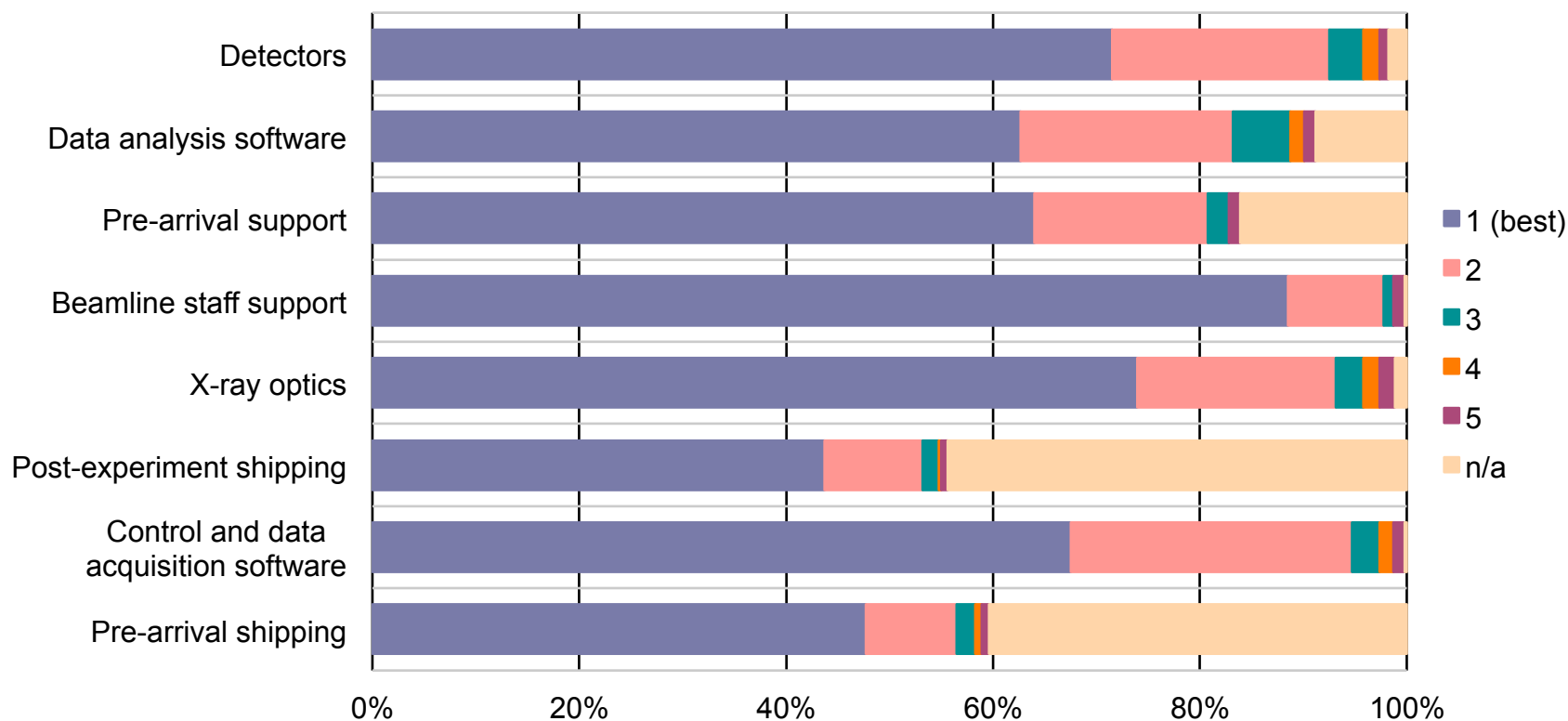
--Run was good. We'd like to get a return on our missing hour of beam time due to the shift to daylight savings time :)
More seriously, it would be nice to have a shield on the LN2 ports (aka a piece of rubber hose) of the 7 T magnet to keep the BNCs from freezing and icing up resulting in poor/sporadic electrical contact from the electron yield detector to the preamp. Silly problem that took us by surprise and took a while to diagnose.

--To whom it may concern: the high-rep rate system at 7ID-D is unique, and when operated in combination with the high flux available from the APS and 7ID it provides unparalleled measurement possibilities...Because of the stable technical installation, setup for these experiments is straightforward and routine, so I would recommend considering allocating a smaller number of measurement shifts for beamtimes (e.g. 3 days) and increase the number of beamtime allocations.

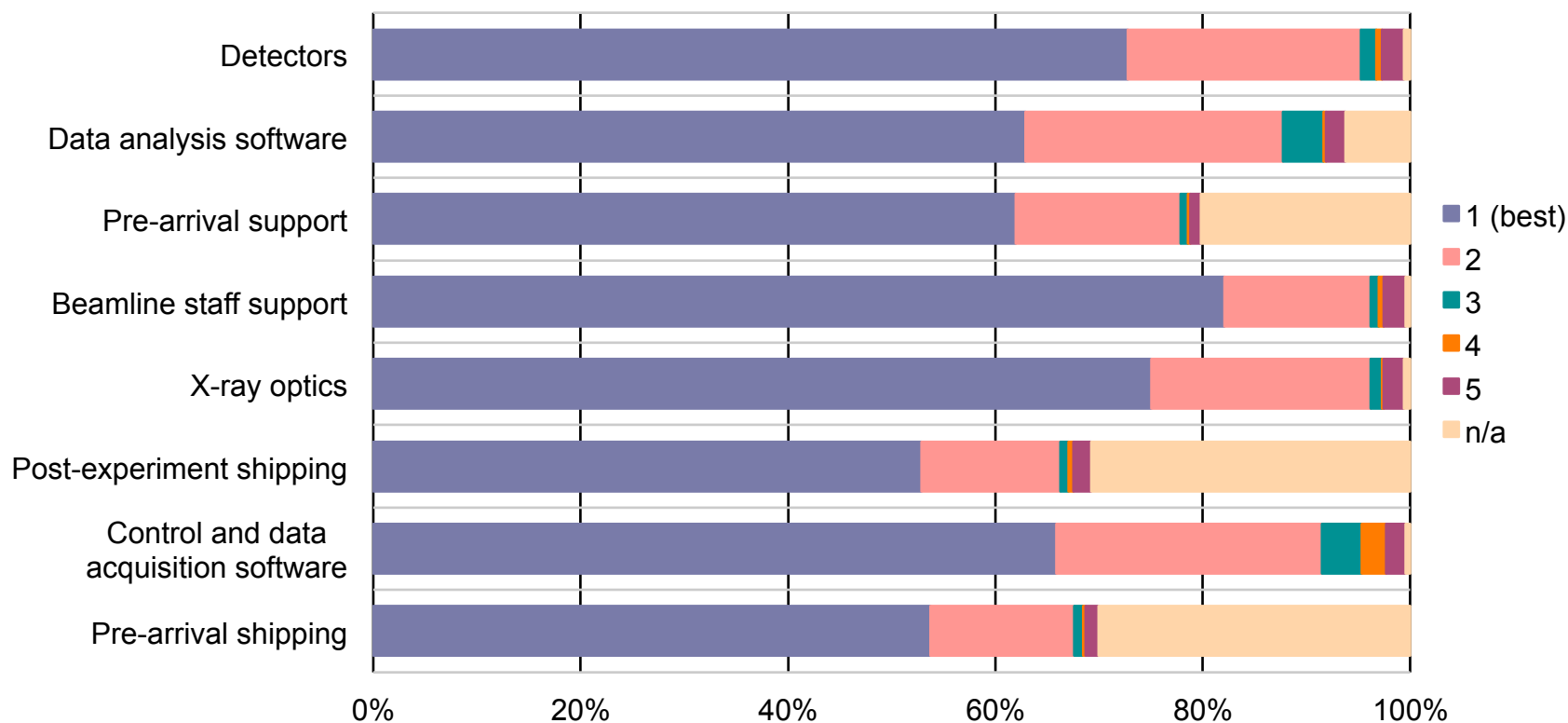
--It would be good to know when a badge needs to be renewed. We obtained gate passes that expired on the day of our arrival (!). One of us had to wait at the entrance gate for 1.5 hours just to get back to the Guest House, because of the gate pass expiration.



Response to Mandatory Questions - XSD Beamlines



Response to Mandatory Questions - non-XSD Beamlines





Sample of beamline specific questions

Did you make use of our online videos?

What other topics would you like to see covered by a tutorial video?

What type of support was provided by the beamline staff?

What would you prioritize for future improvements at the beamline?

What advice would you share with other 11-ID-B users?



Host Assignments for Foreign Nationals Today

- Registration form submitted to APS
- 593 request prepared and submitted to FAVOR for foreign nationals access approval
 - Host currently assigned to 593 by User Office
 - Primary beamline scientist for first choice beamline on a GUP, or
 - S. White-DePace if no GUP is in place



Host Assignments for Foreign Nationals Going Forward

- Group leaders and/or CAT directors will identify beam line staff that will host experiments on their beamline
- Individuals will be given a JHQ for host training
 - Yearly requirement
 - Argonne training system will send auto reminders for retraining



Host Assignments for Foreign Nationals Going Forward

- Beamline safety review staff will identify host on all ESAFs
 - New host field will be added to ESAF
 - Trained hosts for each beamline will automatically appear on dropdown menu in new host field
 - Untrained hosts can be added to ESAF form easily
 - User Office will be notified and will ensure training is taken
 - Host information for foreign nationals will be automatically uploaded to FAVOR (DOE Order requirement)
 - Hosts of foreign nationals will receive a notification e-mail of who they are hosting and when
 - All data will be uploaded to the User Office data base and used for future projects (host will be added to the EEFs, host portal tool)



Questions?

